Introduction to OMFIT for the 2014 OMFIT-BOUT++ workshop

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DIII-D NATIONAL FUSION FACILITY

GENERAL ATOMICS

One Modeling Framework for Integrated Tasks

OMFIT is an integrated modeling framework that:

1. **Enables codes to interact in complicated workflows**
   Managing complexity of data exchange and codes execution

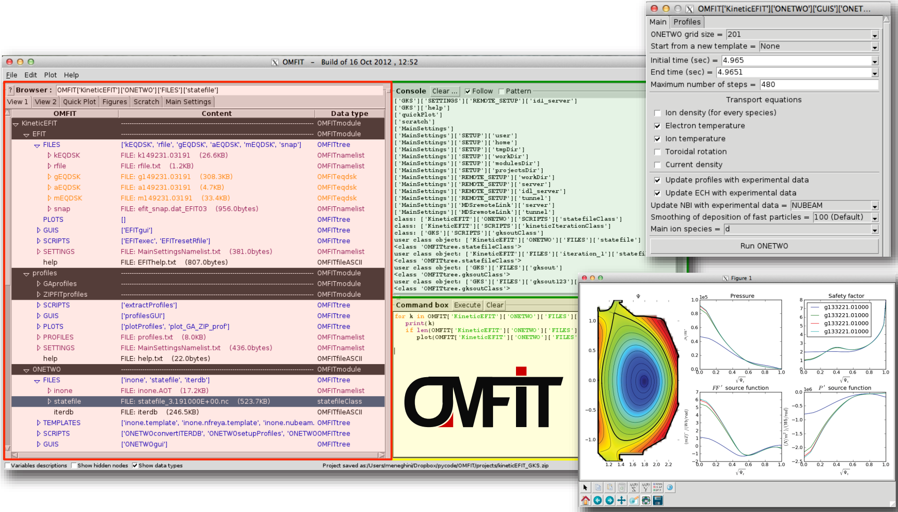
2. **Facilitates all aspects of the entire modeling cycle**

   Development → Verification & Validation → Analysis & Prediction

   Not only execution, but also simulation setup, debugging, comparison with other codes and experiments, data managment, post-processing and plotting, ...

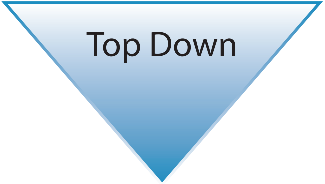
How? OMFIT is an hybrid between a workflow manager and an integrated development environment (IDE)

O. Meneghini and L. Lao, Plasma and Fusion Research, **8** 2403009 (2013)



OMFIT is unique in its integration approach

Most frameworks start from the overall integration process

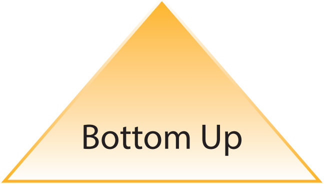


Pros
- Consistent solution

Cons
- Strict rules and protocols
- Hard to build (foresight)
- Hard to change
- Expensive
- Imposed process

Integrate components based on experience and expectations

Integrate components in ways that could not be anticipated



OMFIT starts from individual projects

Pros
- Looser rules and protocols
- Easy to build (incremental)
- Easy to change
- Cost effective
- Grassroots process

Cons
- Uncoordinated solutions

The centerpiece of OMFIT is its flexible data structure

The **OMFIT-tree** is a hierarchical, self-descriptive data structure that enables data exchange among different codes

- Collect data independently of its origin and type
- Objects' content appear in their subtree
- No a-priori decision of what is stored and how
- Codes exchange data by referring quantities in the tree

Same functionality as the "statefile" structures of other frameworks...

...but **free-form !**

Like *MDS+* or *file-system* on your own laptop: the data is stored however it is deemed more logical to accomplish a certain task

With N codes, it's an N^2 problem! How is it possible to make all these codes talk to one another?

- By reading/writing a few (10+) standard scientific data formats OMFIT can interact with many different codes
- Often codes need to exchange only small amount of data
- Exploit existing integration efforts:
  - Many codes already accept each others' files
  - Conversion utilities are already available

OMFIT-tree offers many advantages:

- No need to modify codes and their I/O
  - No burden on developers of individual codes
  - Effort done by users interested in integrating
- Skips all-together arguments about which data structure to use
- Survival of the framework does not depend on widespread adoption of its own data structure
- Does not exclude use of data structures from other frameworks

Other important characteristics of the OMFIT framework

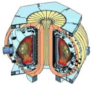
Lightweight, pure-Python framework is easy to install, maintain, and expand

Supports **remote** and **parallel** code execution

Python scripting and **component based approach** allow building of powerful and complex workflows

Graphical user interfaces ease execution of each component and their interaction

Power users retain full control of code I/O files and execution



Integrated with experimental databases for data analysis, generation of code inputs, and validation

Collaborative environment supports distributed development effort, code revision, and collective intelligence

OMFIT provides an increasing list of ever improving modules

Easy to support new codes, especially if they use standard file formats

Equilibrium

EFIT
VARYPED
CORSICA

Exp. analysis

PROFILES
TIMINGS
SCOPE

Gyro-kinetic

GYRO
TGLF
GKS

Transport

ONETWO
NEO
TGYRO
BRAINFUSE

RMP

M3DC1
NTV
FLUTTER
SURFMN

Heating

GENRAY
TORBEAM
NUBEAM

Stability

DCON
GATO
PEST3
ELITE

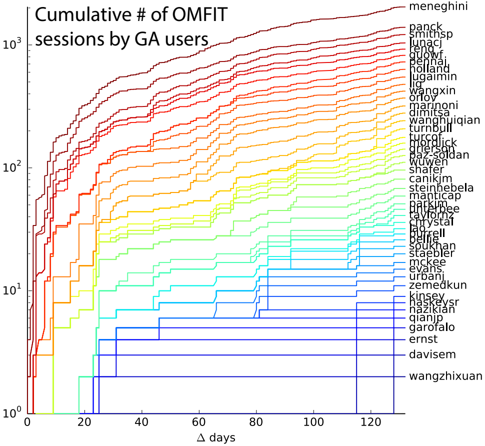
Frameworks

IPS
BOUT++

OMFIT

User adoption and citations are the two most important measures of a framework's success

- Cited in 7 refereed journals
- Used by **60+ users** on the GA servers alone

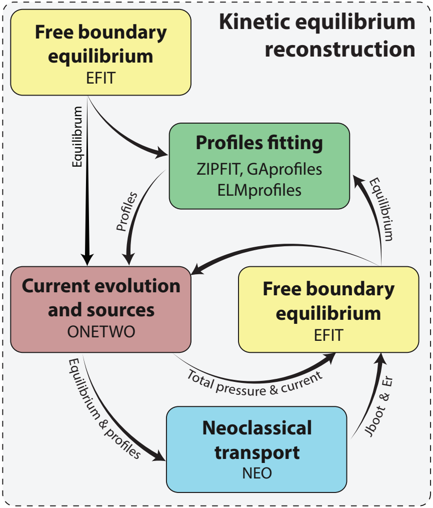


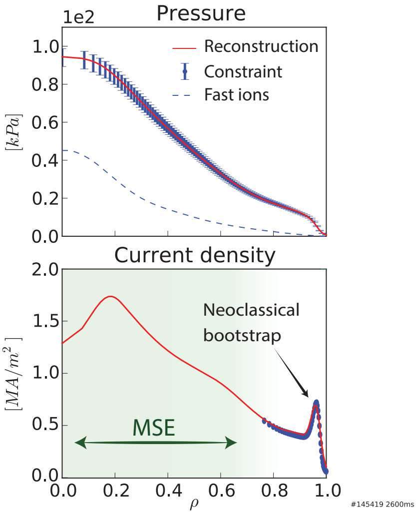
Broad range of applications

- Kinetic EFIT reconstruction
- Core stability calculations
- Edge stability diagrams
- Self-consistent steady state transport simulations
- Self-consistent time-dependent transport simulations
- Neoclassical theory validation
- Validation of Sauter Vs kinetic neoclassical
- Divertor design
- Helicon wave system design
- Validation of magnetic flutter theory
- Validation of neoclassical toroidal viscosity theory
- Building of neural network transport models
- Self-consistent study of interaction between islands and ITG
- Experimental data analysis for transport and 3D fields

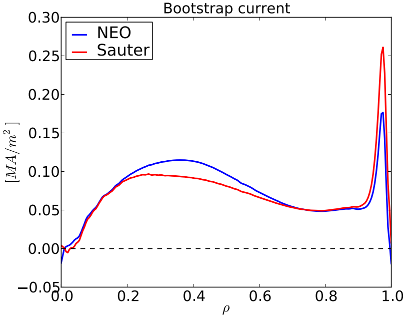
Streamlined DIII-D kinetic EFIT reconstructions

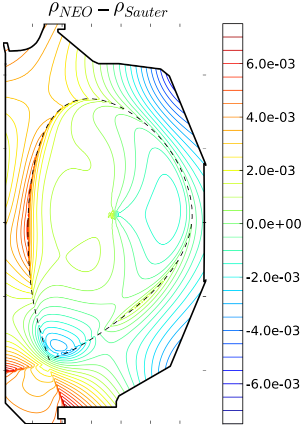
Kinetic equilibria are at the foundation of most DIII-D physics studies





Integrated accurate neoclassical bootstrap current calculation in kinetic-EFIT





- In low collisionality cases, Sauter bootstrap model can be off by as much as 40% from neoclassical calculations (e.g. from NEO)

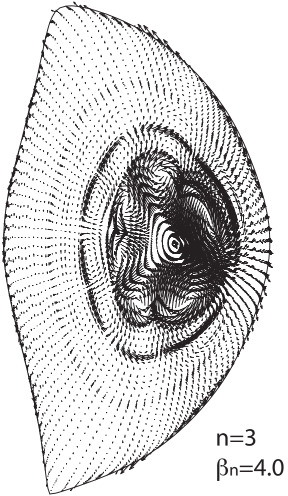
- NEO model leads to significantly lower magnetic χ^2 than Sauter

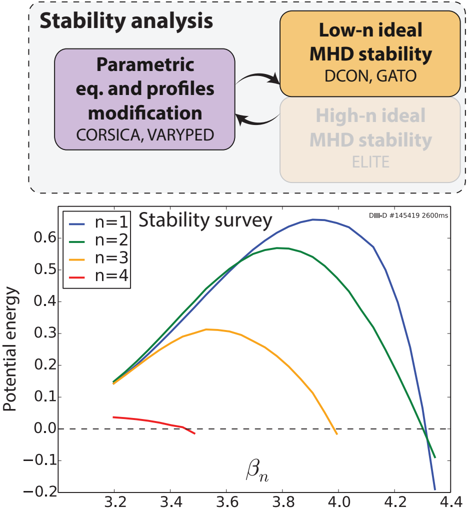
Belli, E. et al., Plasma Physics and Controlled Fusion, **56** 045006 (2014)

Ren, Q. et al., *Test of bootstrap current models using high Beta-p EAST-demonstration plasmas on DIII-D*, Submitted to PPCF

Performed DIII-D core stability analyses

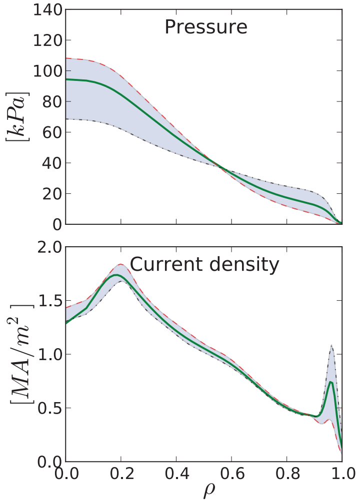
Find stability β limit by scaling equilibrium pressure

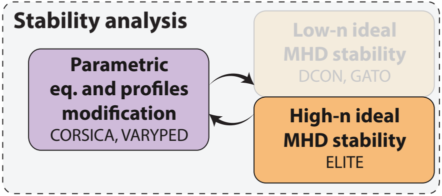


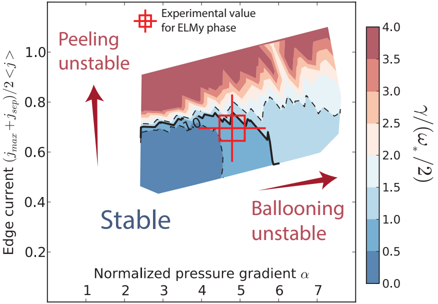


Generated DIII-D edge stability diagrams

Evaluate peeling-ballooning stability as function of edge ∇P and J

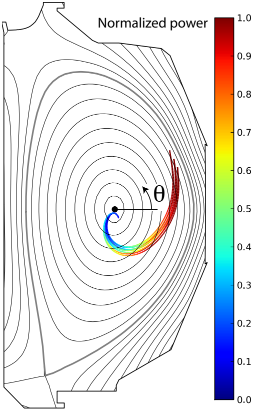


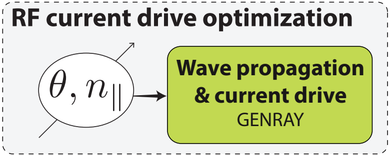


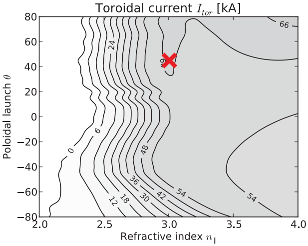


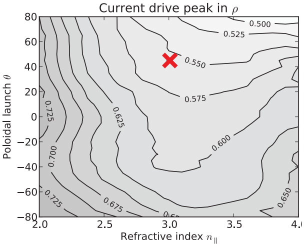
Optimized current drive and radial deposition profile for the proposed DIII-D Helicon wave system

Optimization as a function of $n_{\|}$ and poloidal launch angle





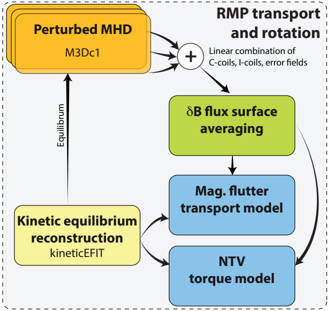


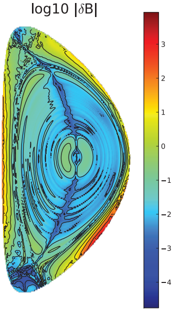


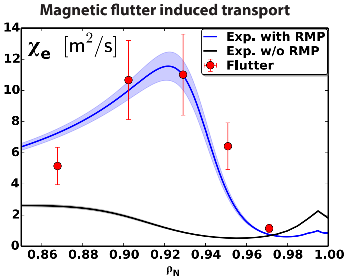
R. Prater et al., Nuclear Fusion, **54** 083024 (2014)

Helped validate magnetic flutter and neoclassic toroidal viscosity theories

- Linear combination of M3D-C1 runs for each of the RMP coil sets
- Flux surface averaging and spectral decomposition within OMFIT
- Implemented both models as OMFIT modules
- Integration with experimental databases allow seamless comparison with experiments





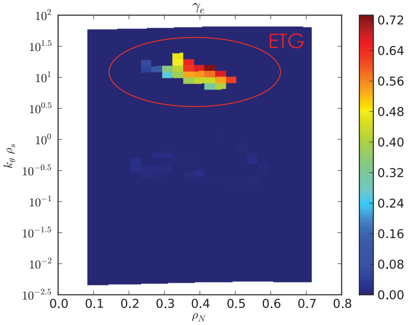


Raum, et al. *Investigating the Validity of the "Magnetic Flutter" Model in the Presence of 3D External Magnetic Fields*, To be published

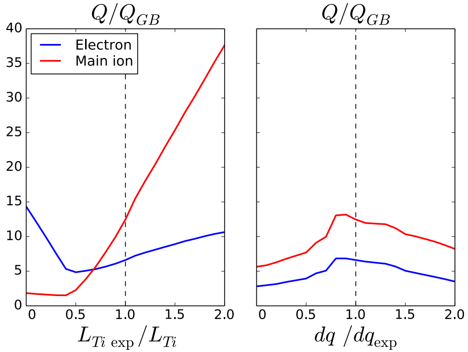
Paz-Soldan et. al *The importance of matched poloidal spectra to error field correction in DIII-D*, Submitted for publication

Interpret transport experiments and conduct sensitivity analyses with TGLF transport model

Control-room kinetic-EFIT and TGLF radial scans to identify mode structures and provide feedback to experiments

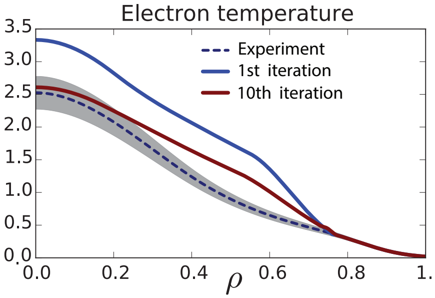


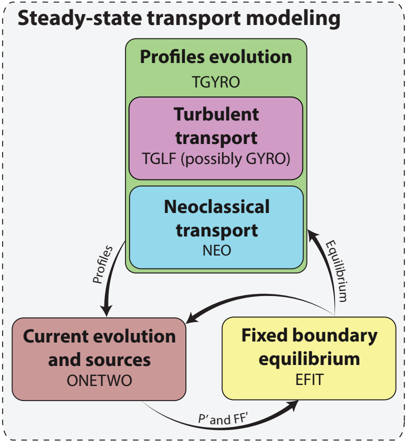
TGLF sensitivity analysis to identify critical gradients and evaluate transport stiffness as function of different plasma parameters



Performed self-consistent steady-state equilibrium/transport studies using first-principles transport models

- Efficient steady state solution by decoupling time-scales
- Important interplay between transport and equilibrium solutions
- Workflow is the basis of recent FNSF scenario development effort

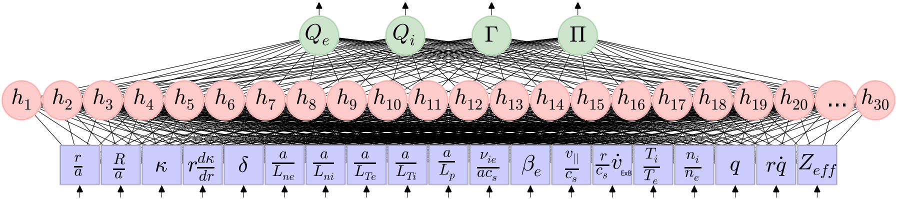




Conceived a fundamentally new approach to address the problem of transport in tokamak plasmas

Use Neural Networks to obtain non-linear multi-dimensional regression of experimentally measured transport

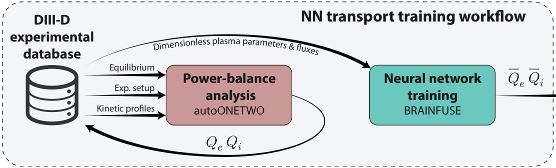
- Output electron and ion heat, particles and momentum fluxes
- Same dimensionless input parameters as first-principles models
- Only assumes that transport is a local phenomenon: $\rho/L \ll 1$

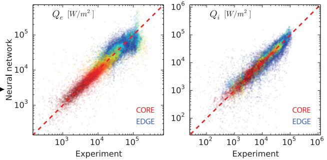


We call it **BRAINFUSE** and it is powered by OMFIT

Meneghini, O. et al., Physics of Plasmas **21** 060702 (2014)

The Neural Network can infer a transport model from the massive volume of aggregated experimental data





Big-data analytics approach is complementary to the development of first-principles theories

Pros

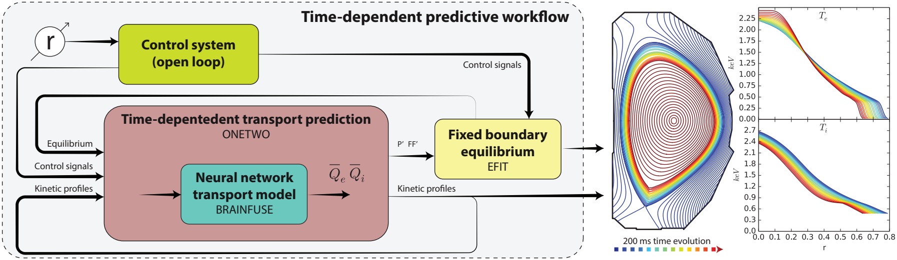
- Very accurate, error is limited by quality of the data
- Computationally efficient ($\sim 10^5\times$ faster than TGLF)

Cons

- Black box model
- Good for interpolation but not extrapolation

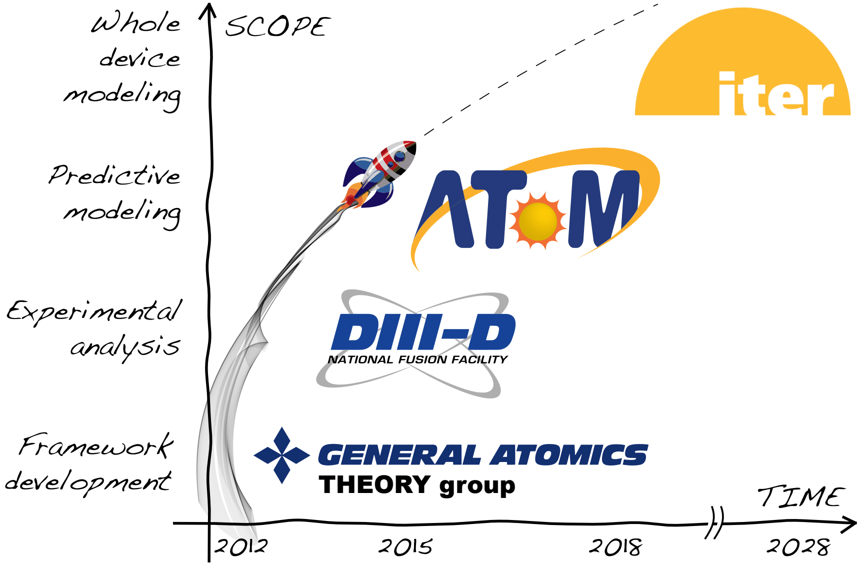
Efficiency of NN transport model enables time-dependent transport-equilibrium evolution studies

Developed BRAINFUSE FORTRAN module and coupled it into ONETWO transport code



- Time-dependent changes to equilibrium and sources, as experimentalists would do during experiments
- 200 ms plasma evolution in $<$10 minutes simulation time
- Possibly a transformational tool for planning of DIII-D shots

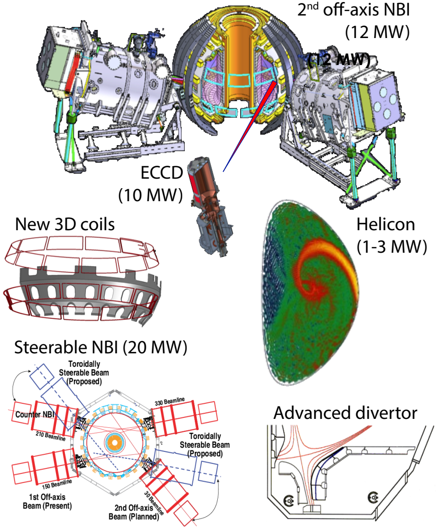
OMFIT is boosting a long-term vision for the GA integrated modeling effort



Strive for a stronger integration with DIII-D

- Continue support of DIII-D operations and experimental analyses
- Assist components design for extensive upgrades plan
- Validate edge modeling codes with experiment
- Develop new burning plasma and non-inductive scenarios with power upgrades
- Provide the tools to predict FNSF performance and accelerate its design

DIII-D 2015 → 2025 upgrade vision



Advanced Tokamak Modeling will boost predictive capabilities and broaden community engagement

3 years SciDAC project starting now:

> *"To enhance and extend present modeling capabilities, by supporting, leveraging, and integrating existing research"*

GENERAL ATOMICS

OAK RIDGE National Laboratory

UCSD

Lawrence Livermore National Laboratory

FASTMATH

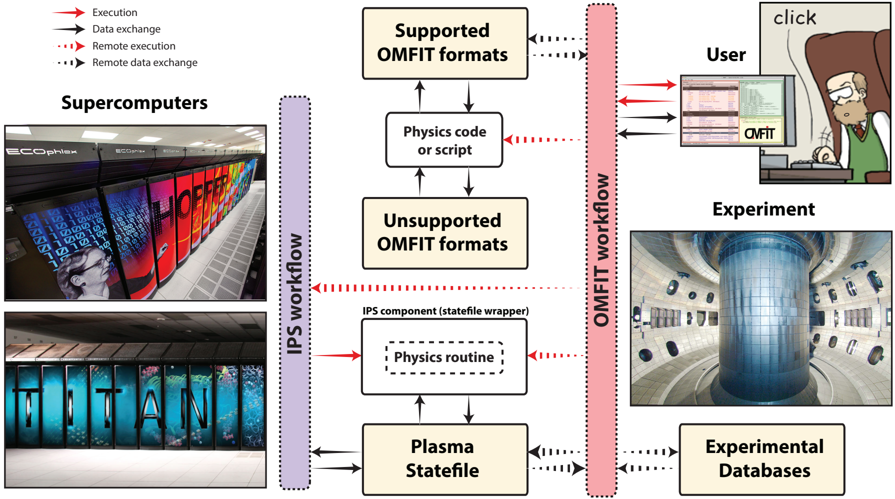
SUPER

1. Bridge gap between *experimental data analysis* and *high performance simulation* communities
2. Performance engineering of critical HPC components
3. Study coupled core, pedestal, and scrape-off layer physics

Coupling OMFIT to IPS provides streamlined HPC modeling capabilities to fusion scientists

IPS focuses on solving challenging computational problems

OMFIT focuses on experimental analysis and convenient user interface

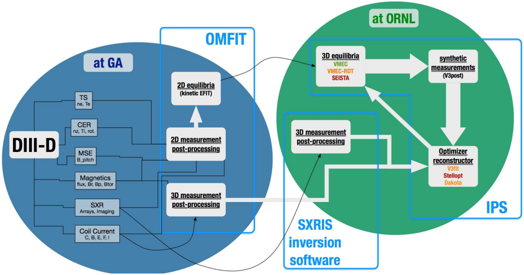


Coupling OMFIT and IPS will also combine users bases and expand the list of available physics codes

AToM will match the needs of:

- Computer scientists looking for users to productively use their systems
- Fusion scientist needing quick turnaround for analyses of increasing complexity

e.g. 3D EQ reconstruction



OMFIT

EFIT
GATO
GENRAY
GKS
ITMactor
PEST3
SURFMN
TGLF
TORBEAM

BOUT++
M3Dc1

ONETWO

GLF23
NUBEAM
MMM
GENRAY

TGYRO

NEO
GYRO
TGLF

IPS

CQL3D
GENRAY
ROTEQ
TORIC

AORSA
NUBEAM

CORSICA

CORSICA-EQ
GLF23
DCON

FASTRAN

GLF23
MMM
TGLF
NCLASS

TSC

GLF23
NCLASS
TSC-EQ

Planned:

C2	NEO3D	COGENT
EPED	SOLPS	NIMROD
LE3	VMEC	UEDGE

Designed generic OMFIT→IPS interface by taking advantage of predefined structure of IPS simulation

Two new OMFIT modules:

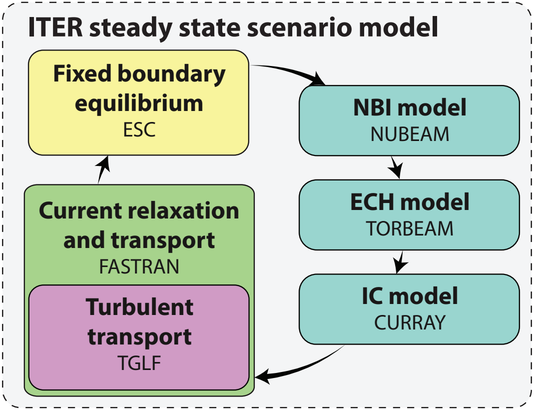
- **IPScore**: manages IPS config file and execution
- **IPSworkflow**: extracts workflow from existing IPS simulation
  1-to-1 correspondance between OMFIT modules and IPS components

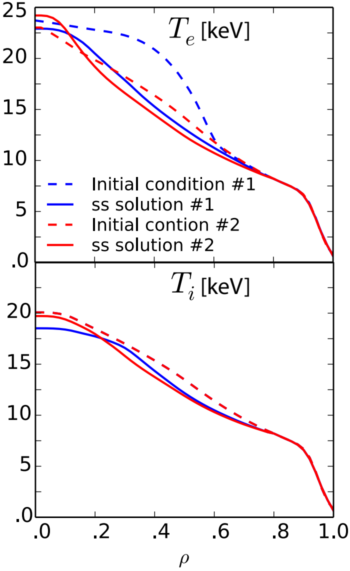
OMFIT→IPS interface allows:

- **Pre-processing**
  - Start from existing IPS run
  - Users setup simulations using GUIs
  - Power users retains ability to change every aspect of the simulation
- **Execution** simulations on different HPC systems
- **Post-processing**
  - Users use pre-defined summary plots
  - Power users have total freedom to slice and dice output data
  - Analyze data also from existing IPS runs

Coupling between OMFIT and IPS demonstrated for ITER steady-state scenario development workflow

Stable transport solution starting from two very different initial conditions for T_e





Accomplishing AToM goals will give OMFIT strong credibility to make a significant contribution to ITER

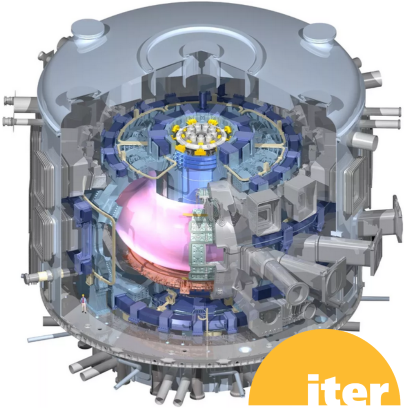
ITER-IMAS mimics EU-ITM framework using Kepler as workflow manager and Consistent Phisical Objects (CPOs) as data structures

ITER is committed to its data structure but not to the framework

- Likely that ITER will allow use of frameworks from different institutions

Natural selection will favor the best integrated modeling solution

- Need to interface OMFIT with ITER-IMAS data structure
- **User adoption and scientific impact will define our success**



Conclusions

- Developed the OMFIT integrated modeling framework for GA
- Performed equilibrium, stability, H&CD and transport studies
- Conceived a fundamentally new neural-network transport model

These premises set the basis for:

- A stronger integration with DIII-D
- Extension of predictive capabilities with the AToM project
- Contribute to the ITER modeling program

A strong IM program is crucial for US/world fusion

OMFIT provides the infrastructure to channel our common efforts